

IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 4. C₆H₁₄ Hydrocarbons with Water

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The mutual solubility and related liquid–liquid equilibria of C₆H₁₄ hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determination of solubility in five chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For all five systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of the all experimental data for a given homologous series of saturated or unsaturated aliphatic hydrocarbons was used. © 2005 American Institute of Physics.
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Key words: C₆H₁₄ hydrocarbons; critical evaluation; heavy water; liquid–liquid equilibria; solubilities; water.

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1. Preface

1.1. Scope of This Volume

This paper is Part 4 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms.^{1,2} This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations reported solubility values are characterized as Recommended, Tentative, Doubtful, or Rejected, based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.^{3–6} Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, the derivation of the smoothing equations used calculate reference values, and the scope of the Solubility Data Series can be found in Part 1 (Maczynski and Shaw⁶).

1.2. References for the Preface

- ¹D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 37, *Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C₅ to C₇* (Pergamon Press, New York, 1989).
- ²D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 38, *Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C₈ to C₃₆* (Pergamon Press, New York, 1989).
- ³A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, *Monatshefte für Chemie* **134**, 633 (2003).
- ⁴A. Maczynski, B. Wisniewska-Goclowska, and M. Goral, Recommended Liquid-Liquid Equilibrium Data, Part 1: Binary C₅–C₁₁ Alkane-Water Systems, *J. Phys. Chem. Ref. Data* **33**(2), 549 (2003).
- ⁵M. Goral, B. Wisniewska-Goclowska, and A. Maczynski, Recommended Liquid-Liquid Equilibrium Data, Part 2: Binary Unsaturated Hydrocarbon-Water Systems *J. Phys. Chem. Ref. Data* **33**(2), 579 (2003).
- ⁶A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series, *Hydrocarbons with Water and Seawater—Revised and Updated, Part 1. C₅ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **34**(1), 657 (2005).

2. Introduction to the Solubility Data Series: Solubility of Liquids in Liquids

2.1. Nature of the Project

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

This series is concerned primarily with liquid-liquid systems, but a limited number of related solid–liquid, fluid–fluid, and multicomponent (organic–water–salt) systems are included where it is considered logical and appropriate. Solu-

bilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

2.2. Compilations and Evaluations and Quantities and Units Used in Compilation and Evaluation of Solubility Data

Formats for the compilations and critical evaluations have been standardized for all volumes, and complete details for these formats can be found in previous *Solubility Data Series* volumes, for example, Sazonov and Shaw.¹

Solubilities of liquids in liquids and solids in liquids have been the subject of research for a long time, and have been expressed in a great many ways. The nomenclature, use of symbols and units in the *IUPAC-NIST Solubility Data Series* follow, where possible, Mills,² again reviewed in detail in Sazonov and Shaw.¹ A few quantities follow the ISO standards³ or the German standard;⁴ see a review by Cvitaš⁵ for details. Updated definitions on nomenclature and use of symbols and units has been published in a recent review by Lorimer.⁶

A note on nomenclature. The nomenclature of the IUPAC *Green Book*² calls the solute component B and the solvent component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the *Green Book*. Additional details can be found in the review by Lorimer.⁶

2.3. References for the Introduction to the Solubility of Liquids in Liquids

- ¹V. P. Sazonov and D. G. Shaw, eds., *Acetonitrile Binary Systems*, IUPAC-NIST Solubility Data Series, Vol. 79, *J. Phys. Chem. Ref. Data* **31**(4), 989 (2002).
- ²I. Mills, et al., eds., *Quantities, Units and Symbols in Physical Chemistry*, the *Green Book* (Blackwell Scientific Publications, Oxford, UK, 1993).
- ³ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).
- ⁴German Standard, DIN 1310, *Zusammensetzung von Mischphasen* (Beuth Verlag, Berlin, 1984).
- ⁵T. Cvitaš, *Chem. International* **17**(4), 123 (1995).
- ⁶J. W. Lorimer, *Quantities, Units and Conversions*, in G. T. Hefter and R. P. T. Tomkins, eds., *The Experimental Determination of Solubilities* (Wiley, New York, 2003).

3. C₆ Hydrocarbons with Water

3.1. 2,2-Dimethylbutane*

References:

- Components:
 (1) 2,2-Dimethylbutane; C₆H₁₄; [75-83-2]
 (2) Water; H₂O; [7732-18-5]
- Evaluators:
 A. Maczynski, M. Goral, and B. Wisniewska-Groclowska,
 Thermodynamics Data Center, Warsaw, Poland, July, 2003.

Critical Evaluation of the Solubility of 2,2-Dimethylbutane (1) in Water (2)

The experimental solubility for (1) in (2) has been investigated by McAuliffe¹ at 298 K, Polak and Lu² at 273 K and 298 K, and Price³ at 298 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + \Delta_{\text{sl}} C_P / R [T_{\min}/T - \ln(T_{\min}/T) - 1]. \quad (1)$$

where: $\ln x_{\min,1} = -12.52$; $\Delta_{\text{sl}} C_P/R = 43.0$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 1. The data of McAuliffe, Polak and Lu² and Price³ at 298 K are in good agreement with each other and with 30% relative standard deviation and are Recommended. The data of Polak and Lu² at 273 K are in poor agreement with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in Dimethylbutane (1)

Polak and Lu² investigated the experimental solubility for (2) in (1) at 273 K and 298 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where: $d_1 = -1.299$; $d_2 = -6.468$; $d_3 = -0.056$; $d_4 = -7.484$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 2,2-dimethylbutane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 2. The data of Polak and Lu² at 273 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Polak and Lu² at 298 K are in poor agreement with the reference data and are Doubtful.

TABLE 1. Experimental values for solubility of 2,2-dimethylbutane (1) in water (2)

T/K	Experimental values x_1 (R=recommended, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$8.23 \cdot 10^{-6}$ (D; Ref. 2)	$5.4 \cdot 10^{-6}$
298.2	$3.85 \cdot 10^{-6}$ (R; Ref. 1), $4.97 \cdot 10^{-6}$ (R; Ref. 2), $4.43 \cdot 10^{-6}$ (R; Ref. 3)	$4.1 \cdot 10^{-6}$

TABLE 2. Experimental values for solubility of water (2) in 2,2-dimethylbutane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	$1.53 \cdot 10^{-4}$ (T; Ref. 2)	$2.0 \cdot 10^{-4}$
298.2	$4.02 \cdot 10^{-4}$ (D; Ref. 2)	$7.0 \cdot 10^{-4}$

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliiga⁴ are independent data. Therefore these data are Rejected.

Components:		Original Measurements:		Original Measurements:	
(1) 2,2-Dimethylbutane; C ₆ H ₁₄ ; [75-83-2]		(1) 2,2-Dimethylbutane; C ₆ H ₁₄ ; [75-83-2]		J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).	
(2) Water; H ₂ O; [7732-18-5]		(2) Water; H ₂ O; [7732-18-5]			
Prepared By:		Prepared By:		Prepared By:	
M. C. Haulait-Pirson		M. C. Haulait-Pirson		M. C. Haulait-Pirson	
Variables:		Variables:		Variables:	
One temperature: 25 °C		Temperature: 0 °C–25 °C		Temperature: 0 °C–25 °C	
Experimental Data		Experimental Data		Experimental Data	
The solubility of 2,2-dimethylbutane in water at 25 °C was reported to be 18.4 mg(1)/kg sln (0.00184 g(1)/100 g sln). The corresponding mole fraction, x_1 , calculated by the compiler, is 3.85 · 10 ⁻⁶ . The same value is also reported in McAuliffe, ^{1,2}		Solubility of 2,2-dimethylbutane in water		Solubility of 2,2-dimethylbutane in water	
		$t/^\circ\text{C}$		$10^6 \cdot x_1$ (compiler)	
		0 ^a		8.23	39.4 ^c
		25 ^b		4.97	23.8 ^c
				Solubility of water in 2,2-dimethylbutane	
		$t/^\circ\text{C}$		$10^4 \cdot x_2$ (compiler)	
		0 ^a		1.53	32 ^d
		25 ^b		4.02	84 ^e
^{a–e} See Estimated Error.		Auxiliary Information		Auxiliary Information	
Method/Apparatus/Procedure:		Source and Purity of Materials:		Source and Purity of Materials:	
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.		(1) Phillips Petroleum Co.; 99+ % purity; used as received. (2) Distilled.		(1) Phillips Petroleum Co.; pure grade reagent 99+ %; shaken three times with distilled water. (2) Distilled.	
Estimated Error:		References:		Estimated Error:	
Temperature: ±1.5 °C. Solubility: 1.3 mg(1)/kg sln (std. dev. of mean).		¹ C. McAuliffe, Nature (London) 200 , 1092 (1963). ² C. McAuliffe, Ann. Chem. Soc. Div. Petrol. Chem. 9 , 275 (1964).		Temperature: (a) ±0.02 °C; (b) ±0.01 °C. Solubility: (c) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).	

3.2. 2,3-Dimethylbutane*

Components:	Original Measurements:
(1) 2,2-Dimethylbutane; C ₆ H ₁₄ ; [75-83-2]	L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).
(2) Water; H ₂ O; [7732-18-5]	
Prepared By:	
M. C. Haulait-Pirson	
Variables:	
One temperature: 25 °C	

Experimental Data

The solubility of 2,2-dimethylbutane in water at 25 °C and system pressure was reported to be 21.1 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00212 g(1)/100 g sin and 4.43 · 10⁻⁶.

Auxiliary Information

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ± 1 °C.
Solubility: ± 0.3 mg(1)/kg(2).

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperature by use of screw cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Components:	Evaluators:
(1) 2,3-Dimethylbutane; C ₆ H ₁₄ ; [79-29-5]	A. Maczynski, M. Goral, and B. Wisniowska-Gocłowska, Thermodynamics Data Center, Warsaw, Poland, July, 2003.
(2) Water; H ₂ O; [7732-18-5]	
Critical Evaluation of the Solubility of 2,3-Dimethylbutane (1) in Water (2)	

Polak and Lu² investigated the experimental solubility for (1) in (2) at 273 K and 298 K, and Price³ at 298 K–423 K. Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + \Delta_{\sin} C_P / R[T_{\min}/T - \ln(T_{\min}/T) - 1], \quad (1)$$

where: $\ln x_{\min,1} = -12.57$; $\Delta_{\sin} C_P / R = 43.3$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 3 and shown in Fig. 1. The data of Polak and Lu,² and Price³ at 298 K are in good agreement with each other and with the reference data (within 30% relative standard deviation) and are Recommended. The data of Price³ at 313 K–423 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Polak and Lu² at 273 K are in poor agreement with the reference data and are Doubtful.

TABLE 3. Experimental values for solubility of 2,3-dimethylbutane (1) in water (2)

T/K	Experimental values x_1		Reference values $x_1 \pm 30\%$
	(R=recommended, T=tentative, D=doubtful)	(R=recommended, T=tentative, D=doubtful)	
273.2	6.87 · 10 ⁻⁶ (D; Ref. 2)	5.1 · 10 ⁻⁶	
298.2	4.70 · 10 ⁻⁶ (R; Ref. 2), 3.99 · 10 ⁻⁶ (R; Ref. 3)	3.8 · 10 ⁻⁶	
313.3	4.01 · 10 ⁻⁶ (T; Ref. 3)	3.8 · 10 ⁻⁶	
328.3	4.95 · 10 ⁻⁶ (T; Ref. 3)	4.2 · 10 ⁻⁶	
372.3	8.38 · 10 ⁻⁶ (T; Ref. 3)	8.2 · 10 ⁻⁶	
394.5	1.19 · 10 ⁻⁵ (T; Ref. 3)	1.4 · 10 ⁻⁵	
410.5	2.05 · 10 ⁻⁵ (T; Ref. 3)	2.1 · 10 ⁻⁵	
422.8	3.37 · 10 ⁻⁵ (T; Ref. 3)	2.9 · 10 ⁻⁵	

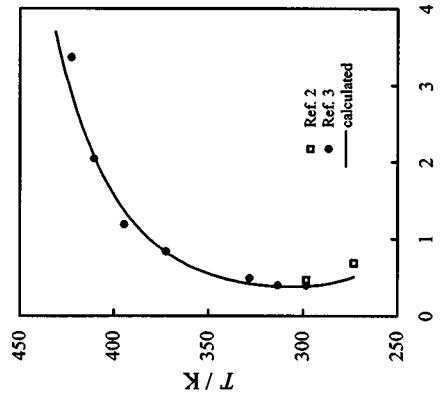


Fig. 1. All the solubility data for 2,3-dimethylbutane (1) in water (2).

Rejected and Inaccessible Data

Critical Evaluation of the Solubility of Water (2) in 2,3-Dimethylbutane (1)
 Englin *et al.*¹ investigated the experimental solubility for (2) in (1) at 273 K–323 K, and Polak and Lu² at 273 K and 298 K. Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^3 + d_4(1 - T_r) \quad (2)$$

where: $d_1 = -1.219$; $d_2 = -6.291$; $d_3 = -0.091$; $d_4 = -4.950$; $T_r = T/493.7$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of 2,3-dimethylbutane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 4 and shown in Fig. 2. The data of Englin *et al.*¹ and Polak and Lu² at 273 K are in good agreement with each other and with the reference data (within 30% relative standard deviation) and are Recommended. The data of Englin *et al.*¹ at 283 K–313 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Englin *et al.*¹ at 323 K and Polak and Lu² at 298 K are in poor agreement with the reference data and are Doubtful.

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szelić⁴ are independent data. Therefore these data are Rejected.

References:

¹B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pyranishnikova, Khim. Tekhnol. Topl. Masei **10**, 42 (1965).

²J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).

³L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

⁴T. Krzyzanowska and J. Szelić, Nauka (Katowice) **12**, 413 (1978).

TABLE 4. Experimental values for solubility of water (2) in 2,3-dimethylbutane (1)

T/K	Experimental values x_2		Reference values $x_2 \pm 30\%$
	(R=recommended, T=tentative, D=doubtful)		
273.2	1.43·10 ⁻⁴ (R; Ref. 2), 1.40·10 ⁻⁴ (R; Ref. 1)		1.9·10 ⁻⁴
283.2	2.80·10 ⁻⁴ (T; Ref. 1)		3.1·10 ⁻⁴
293.2	5.26·10 ⁻⁴ (T; Ref. 1)		5.0·10 ⁻⁴
298.2	4.30·10 ⁻⁴ (D; Ref. 2)		6.3·10 ⁻⁴
303.2	9.18·10 ⁻⁴ (T; Ref. 1)		7.8·10 ⁻⁴
313.2	1.54·10 ⁻³ (T; Ref. 1)		1.2·10 ⁻³
323.2	2.46·10 ⁻³ (D; Ref. 1)		1.8·10 ⁻³

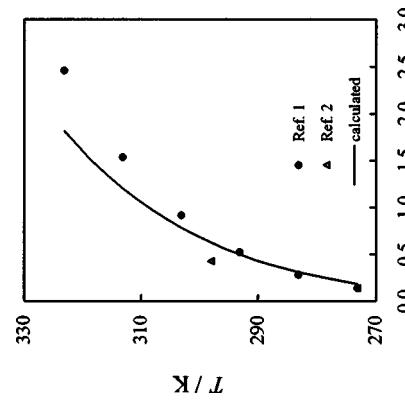


Fig. 2. All the solubility data for water (2) in 2,3-dimethylbutane (1).

Components:		Original Measurements:		Original Measurements:	
(1) 2,3-Dimethylbutane; C ₆ H ₁₄ ; [79-29-8]	B. A. Erigin, A. F. Plaie, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).	(1) 2,3-Dimethylbutane; C ₆ H ₁₄ ; [79-29-8]	J. Polak and B. C.-Y. Lu, Can. J. Chem. 51 , 4018 (1973).	(2) Water; H ₂ O; [7732-18-5]	J. Polak and B. C.-Y. Lu, Can. J. Chem. 51 , 4018 (1973).
Variables:	Prepared By:	Variables:	Prepared By:	Variables:	Prepared By:
Temperature: 0 °C–50 °C	A. Maczynski and M. C. Haulait-Pirson	Temperature: 0 °C–25 °C	M. C. Haulait-Pirson	Temperature: 0 °C–25 °C	M. C. Haulait-Pirson
Experimental Data		Experimental Data		Experimental Data	
Solubility of water in 2,3-dimethylbutane		Solubility of water in 2,3-dimethylbutane		Solubility of 2,3-dimethylbutane in water	
t/°C	10 ⁴ ·x ₂ (compiler)	t/°C	10 ⁶ ·x ₁ (compilers)	t/°C	mg(1)/kg sln mg(2)/kg sln
0	1.4	0.0029	0 ^a	6.87	32.9 ^c
10	2.8	0.0058	25 ^b	4.70	22.5 ^c
20	5.26	0.0110			
30	9.18	0.0192			
40	15.4	0.0323			
50	24.6	0.0516	t/°C	10 ⁴ ·x ₂ (compiler)	mg(2)/kg sln
Auxiliary Information		Auxiliary Information		Auxiliary Information	
Source and Purify of Materials:		Source and Purify of Materials:		Source and Purify of Materials:	
(1) Not specified.		(1) Not specified.		(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.	
(2) Not specified.		(2) Not specified.		(2) Distilled.	
Estimated Error:		Estimated Error:		Estimated Error:	
Not specified.		Not specified.		Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C.	
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was determined.		Concentration: (a) ± 1.7%; (b) ± 4.7%; (c) ± 3.1% (mean).		Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).	
Method/Apparatus/Procedure:		Method/Apparatus/Procedure:		Method/Apparatus/Procedure:	
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was determined.		The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and held in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.		The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and held in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.	
Source and Purify of Materials:		Source and Purify of Materials:		Source and Purify of Materials:	
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.		(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.		(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.	
(2) Distilled.		(2) Distilled.		(2) Distilled.	
Estimated Error:		Estimated Error:		Estimated Error:	
Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C.		Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).		Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C.	
Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).		Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).		Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).	

3.3. Hexane*

Components:	Original Measurements:			
(1) 2,3-Dimethylbutane; C ₆ H ₁₄ ; [79-29-8]	L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).			
(2) Water; H ₂ O; [7732-18-5]				
Prepared By:				
F. Kapuku				
Variables:				
Temperature: 25 °C–149.5 °C				
Experimental Data				
Solubility of 2,3-dimethylbutane in water at system pressure				
$10^6 \cdot x_1$				
$t/^\circ\text{C}$				
25.0	3.99	0.00191		
40.1	4.01	0.00192		
55.1	4.95	0.00237		
99.1	8.38	0.00401		
121.3	11.87	0.00568		
137.3	20.46	0.00979		
149.5	35.75	0.01710		
Auxiliary Information				
Source and Purity of Materials:				
(1) Phillips Petroleum Company; 99%.				
(2) Distilled.				
Estimated Error:				
Temperature: ± 1 °C.				
Solubility: range of values given above.				
Method/Apparatus/Procedure:				
Room-temperature solubility were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase.				
High-temperature solubility work was carried out in the oven of a gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.				

Evaluators:		
A. Maczynski, M. Goral, and B. Wisniewska-Gocłowska, Thermodynamics Data Center, Warsaw, Poland, July, 2003.		
Critical Evaluation of the Solubility of Hexane (1) in Water (2)		
The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with the ranges of temperature and pressure, if reported.		
Author (s)	T/K	Author (s)
Aquan-Yuen <i>et al.</i> ¹	298	Leinonen and Mackay ⁹
Barone <i>et al.</i> ²	298	Mackay <i>et al.</i> ²¹
Budantseva <i>et al.</i> ⁶	293	McAuliffe ²²
Durand ¹⁰	289	McBain and Lissant ²³
Filner ¹²	289	McCants <i>et al.</i> ²⁴
Jones and McCants ¹³	311	Nelson and De Ligny ²⁵
Jonsson <i>et al.</i> ¹⁴	288–308	Polak and Lu ²⁷
Korenman and Aref ^{eval 15}	293	Price ²⁸
Korenman and Aref ^{eval 16}	298	Tewari <i>et al.</i> ³⁴
Krasnoshchekova and Gubergits ¹⁷	298	Tsonopoulos <i>et al.</i> ³⁵
	311–473	(348–3516 kPa)
Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:		
$\ln x_1 = \ln x_{\min,1} + \Delta_{\text{lin}} C_p / R [T_{\min}/T - \ln(T_{\min}/T)]$,		
where: $\ln x_{\min,1} = -13.04$; $\Delta_{\text{lin}} C_p/R = 45.6$; $T_{\min} = 306\text{ K}$.		
Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data.		
Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 5.		
All the experimental and reference data are listed in Table 6 and shown in Fig. 3. The Recommended and Tentative data are shown in Fig. 4.		
Critical Evaluation of the Solubility of Water (2) Hexane (1)		
The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with the ranges of temperature and pressure, if reported.		
Author (s)	T/K	Author (s)
Benkovski <i>et al.</i> ³	303	Liu <i>et al.</i> ²⁰
Black <i>et al.</i> ⁴	293	Polak and Lu ²⁷
Budantseva <i>et al.</i> ⁶	293	Roddy and Coleman ³⁰
Burd and Braun ⁷	355–478 (207–3241 kPa)	Sugii and Katayama ³²
Charykov <i>et al.</i> ⁸	293–313	Tsonopoulos <i>et al.</i> ³⁵
Englin <i>et al.</i> ¹¹		Zel'venskii <i>et al.</i> ³⁶
Jones and McCants ¹³	298–318	(348–3516 kPa)
Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:		
$\ln x_2 = d_1 + d_2 (1/T_r - 1) + d_3 (1 - T_r)^{1/3} + d_4 (1 - T_r)$,		
where: $d_1 = -1.118$; $d_2 = -6.113$; $d_3 = -0.144$; $d_4 = -5.049$; $T_r = T/499.8$.		
In contrast to the smoothed equation used by Hettler and Young ⁴⁹ for regression of the solubility data of water in hexane, Eq. (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of hexane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 7.		
All the experimental and reference solubility data for (2) in (1) are listed in Table 8 and shown in Fig. 5. The Recommended and Tentative data are shown in Fig. 6.		

TABLE 5. The data categories for solubility of hexane (1) in water (2)

<i>T</i> /K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)	<i>T</i> /K	<i>P</i> /kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)
273.2	Polak and Lu ²⁷	273.2		273.2		$3.44 \cdot 10^{-6}$ (T; Ref. 27)
277.2	Nelson and De Ligny ²⁶	277.2		277.2		$3.42 \cdot 10^{-6}$ (T; Ref. 26)
287.2	Nelson and De Ligny ²⁶	287.2		287.2		$3.17 \cdot 10^{-6}$ (T; Ref. 26)
288.2	Jonsson <i>et al.</i> ¹⁴			288.2		$2.24 \cdot 10^{-6}$ (T; Ref. 14)
288.7				288.7		$2.92 \cdot 10^{-5}$ (D; Ref. 12)
289.2	Fuehner ¹²			289.2		$7.50 \cdot 10^{-6}$ (D; Ref. 10)
293.2	Durand ¹⁰			293.2		$3.00 \cdot 10^{-6}$ (T; Ref. 6), $2.15 \cdot 10^{-6}$ (T; Ref. 14), $2.90 \cdot 10^{-5}$ (D; Ref. 15)
293.2	Korenman and Korenman and Aref <i>et al.</i> ¹⁵	293.2		293.2		$2.57 \cdot 10^{-6}$ (R; Ref. 1), $3.39 \cdot 10^{-6}$ (D; Ref. 2), $2.11 \cdot 10^{-6}$ (R; Ref. 14), $3.30 \cdot 10^{-5}$ (D; Ref. 16), $2.80 \cdot 10^{-6}$ (R; Ref. 17), $2.50 \cdot 10^{-6}$ (R; Ref. 19), $3.40 \cdot 10^{-6}$ (D; Ref. 21), $1.99 \cdot 10^{-6}$ (T; Ref. 22), $2.50 \cdot 10^{-5}$ (D; Ref. 23), $3.83 \cdot 10^{-6}$ (D; Ref. 26), $2.59 \cdot 10^{-6}$ (D; Ref. 27), $1.98 \cdot 10^{-6}$ (T; Ref. 28), $2.58 \cdot 10^{-6}$ (R; Ref. 34)
298.2	Barone <i>et al.</i> ²			298.2		$2.09 \cdot 10^{-6}$ (T; Ref. 14)
298.2	Korenman and Aref <i>et al.</i> ¹⁶ , Mackay <i>et al.</i> ²¹			298.2		$2.11 \cdot 10^{-6}$ (R; Ref. 14), $2.69 \cdot 10^{-6}$ (R; Ref. 26)
298.2	Nelson and De Ligny ²⁶			298.2		$8.30 \cdot 10^{-4}$ (D; Ref. 13), $2.38 \cdot 10^{-5}$ (D; Ref. 35)
298.2	Polak and Lu ²⁷			298.2		$2.00 \cdot 10^{-4}$ (D; Ref. 24)
303.2	Jonsson <i>et al.</i> ¹⁴	303.2		303.2		$2.11 \cdot 10^{-6}$ (T; Ref. 28)
308.2	Jonsson <i>et al.</i> ¹⁴	308.2		308.2		$4.64 \cdot 10^{-6}$ (D; Ref. 26)
308.2	Nelson and De Ligny ²⁶			308.2		$4.42 \cdot 10^{-6}$ (D; Ref. 26)
310.9	Tronopoulos <i>et al.</i> ³⁵	310.9		310.9		$2.76 \cdot 10^{-6}$ (T; Ref. 28)
311.0	Jones and McCants ¹³	311.0		311.0		$3.18 \cdot 10^{-6}$ (T; Ref. 28), $3.22 \cdot 10^{-6}$ (T; Ref. 28)
313.2	McCants <i>et al.</i> ²⁴	313.2		313.2		$5.73 \cdot 10^{-5}$ (D; Ref. 35)
318.1		318.1		318.1		$5.35 \cdot 10^{-5}$ (D; Ref. 35)
328.1	Nelson and De Ligny ²⁶	328.1		328.1		$4.68 \cdot 10^{-6}$ (T; Ref. 28)
328.9	Nelson and De Ligny ²⁶	328.9		328.9		$6.21 \cdot 10^{-5}$ (D; Ref. 35)
328.2	Price ²⁸	328.2		328.2		$6.10 \cdot 10^{-6}$ (T; Ref. 28)
328.9	Price ²⁸	328.9		328.9		$7.86 \cdot 10^{-6}$ (T; Ref. 28)
342.9	Tronopoulos <i>et al.</i> ³⁵	342.9		342.9		$1.19 \cdot 10^{-5}$ (T; Ref. 28)
366.5	Tronopoulos <i>et al.</i> ³⁵	366.5		366.5		$2.71 \cdot 10^{-4}$ (D; Ref. 35)
366.5	Tronopoulos <i>et al.</i> ³⁵	367.6		367.6		$5.6 \cdot 10^{-6}$
367.6		372.2		367.6		$4.9 \cdot 10^{-6}$
372.2	Price ²⁸	373.2		372.2		$5.5 \cdot 10^{-6}$
373.2	Tronopoulos <i>et al.</i> ³⁵	387.5		373.2		$6.10 \cdot 10^{-5}$ (D; Ref. 35)
387.5	Price ²⁸	394.5		387.5		$7.86 \cdot 10^{-6}$ (T; Ref. 28)
394.5	Price ²⁸	410.5		394.5		$9.3 \cdot 10^{-6}$
410.5	Price ²⁸	422.0		410.5		$1.4 \cdot 10^{-5}$
422.0	Tronopoulos <i>et al.</i> ³⁵	423.2		422.0		$2.0 \cdot 10^{-5}$
423.2	Tronopoulos <i>et al.</i> ³⁵	425.0		423.2		$2.1 \cdot 10^{-5}$
425.0		473.2		425.0		$2.32 \cdot 10^{-5}$ (T; Ref. 28)
473.2	Tronopoulos <i>et al.</i> ³⁵			473.2		$1.85 \cdot 10^{-3}$ (D; Ref. 35)

TABLE 6. Experimental values for solubility of hexane (1) in water (2)

<i>T</i> /K	Reference values $x_1 \pm 30\%$
273.2	$3.3 \cdot 10^{-6}$
277.2	$3.0 \cdot 10^{-6}$
287.2	$2.6 \cdot 10^{-6}$
288.2	$2.6 \cdot 10^{-6}$
288.7	$2.6 \cdot 10^{-6}$
289.2	$2.6 \cdot 10^{-6}$
293.2	$2.5 \cdot 10^{-6}$
298.2	$2.4 \cdot 10^{-6}$
303.2	$2.4 \cdot 10^{-6}$
308.2	$2.4 \cdot 10^{-6}$
310.9	$2.4 \cdot 10^{-6}$
311.0	$2.4 \cdot 10^{-6}$
313.2	$2.4 \cdot 10^{-6}$
318.1	$2.4 \cdot 10^{-6}$
328.1	$2.5 \cdot 10^{-6}$
328.9	$2.4 \cdot 10^{-6}$
328.2	$2.4 \cdot 10^{-6}$
328.9	$2.4 \cdot 10^{-6}$
328.9	$2.4 \cdot 10^{-6}$
328.9	$2.4 \cdot 10^{-6}$
342.9	$2.4 \cdot 10^{-6}$
366.5	$2.4 \cdot 10^{-6}$
366.5	$2.4 \cdot 10^{-6}$
367.6	$2.4 \cdot 10^{-6}$
372.2	$2.4 \cdot 10^{-6}$
373.2	$2.4 \cdot 10^{-6}$
387.5	$2.4 \cdot 10^{-6}$
394.5	$2.4 \cdot 10^{-6}$
410.5	$2.4 \cdot 10^{-6}$
422.0	$2.4 \cdot 10^{-6}$
423.2	$2.4 \cdot 10^{-6}$
425.0	$2.4 \cdot 10^{-6}$
473.2	$2.4 \cdot 10^{-6}$

TABLE 7. The data categories for solubility of water (2) in hexane (1)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
273.2	Black <i>et al.</i> ⁴ Chankov <i>et al.</i> ⁸ Englin <i>et al.</i> ¹¹	Polak and Lu ²⁷ Budantseva <i>et al.</i> ⁶	Zelvenskii <i>et al.</i> ³⁶
293.2			Liu <i>et al.</i> ²⁰
298.2		Polak and Lu ²⁷ Roddie and Coleman ³⁰ Sugi and Katayama ³²	
303.0			Benkovskii <i>et al.</i> ³
303.2		Englin <i>et al.</i> ¹¹	Liu <i>et al.</i> ²⁰
308.2			Jones and McCanns ¹³
310.9		Englin <i>et al.</i> ¹¹	
313.2		Tsonopoulos <i>et al.</i> ³⁵	
318.2		Burd and Braun ⁷	Liu <i>et al.</i> ²⁰
354.8		Burd and Braun ⁷	
366.5		Burd and Braun ⁷	
367.6		Burd and Braun ⁷	
373.2		Burd and Braun ⁷	Tsonopoulos <i>et al.</i> ³⁵
379.3		Burd and Braun ⁷	Tsonopoulos <i>et al.</i> ³⁵
394.3		Burd and Braun ⁷	
400.4		Burd and Braun ⁷	
417.6		Burd and Braun ⁷	
422.0		Burd and Braun ⁷	
423.2		Burd and Braun ⁷	
431.5		Burd and Braun ⁷	
442.6		Burd and Braun ⁷	
449.8		Burd and Braun ⁷	
452.6		Burd and Braun ⁷	
460.4		Burd and Braun ⁷	
468.2		Burd and Braun ⁷	
473.2		Burd and Braun ⁷	
477.6		Burd and Braun ⁷	

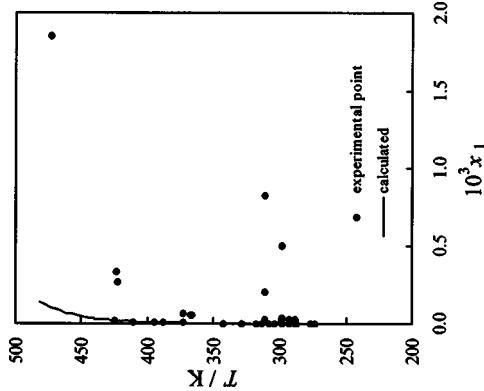


Fig. 3. All the solubility data for hexane (1) in water (2).

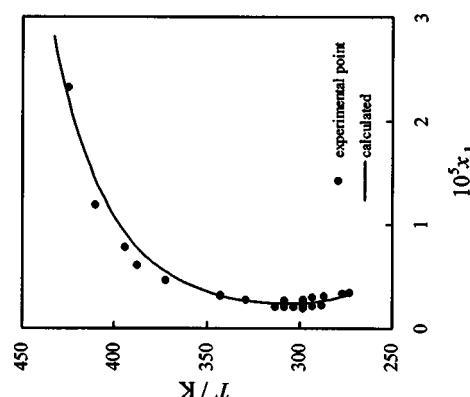


Fig. 4. Recommended and tentative solubility data for hexane (1) in water (2).

TABLE 8. Experimental values for solubility of water (2) in hexane (1)

T / K	P / kPa	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2		$1.34 \cdot 10^{-4}$ (T; Ref. 27)	$1.9 \cdot 10^{-4}$
293.2		$5.30 \cdot 10^{-4}$ (R; Ref. 4), $3.70 \cdot 10^{-4}$ (T; Ref. 6), $4.60 \cdot 10^{-4}$ (R; Ref. 8), $4.83 \cdot 10^{-4}$ (R; Ref. 11), $7.90 \cdot 10^{-4}$ (D; Ref. 36)	$4.9 \cdot 10^{-4}$
298.2		$1.78 \cdot 10^{-2}$ (D; Ref. 20), $4.30 \cdot 10^{-4}$ (T; Ref. 27), $4.76 \cdot 10^{-4}$ (T; Ref. 30), $5.10 \cdot 10^{-4}$ (T; Ref. 32)	$6.1 \cdot 10^{-4}$
303.0		$2.40 \cdot 10^{-4}$ (D; Ref. 3)	$7.6 \cdot 10^{-4}$
303.2		$8.56 \cdot 10^{-4}$ (T; Ref. 11)	$7.6 \cdot 10^{-4}$
308.2		$1.74 \cdot 10^{-2}$ (D; Ref. 20)	$9.5 \cdot 10^{-4}$
310.9		$9.50 \cdot 10^{-3}$ (D; Ref. 11), $1.17 \cdot 10^{-3}$ (R; Ref. 35), $1.23 \cdot 10^{-3}$ (R; Ref. 35)	$1.1 \cdot 10^{-3}$
313.2	45.37 (Ref. 35)	$1.515 \cdot 10^{-3}$ (R; Ref. 35)	$1.2 \cdot 10^{-3}$
318.2		$1.70 \cdot 10^{-2}$ (D; Ref. 20)	$1.4 \cdot 10^{-3}$
354.8	207 (Ref. 7)	$6.70 \cdot 10^{-2}$ (T; Ref. 7)	$5.6 \cdot 10^{-3}$
366.5	414 (Ref. 7)	$1.00 \cdot 10^{-2}$ (T; Ref. 7)	$8.4 \cdot 10^{-3}$
367.6		$5.95 \cdot 10^{-3}$ (D; Ref. 35)	$8.7 \cdot 10^{-3}$
373.2	348.2 (Ref. 35)	$7.09 \cdot 10^{-3}$ (D; Ref. 35)	$1.0 \cdot 10^{-2}$
379.3	689 (Ref. 7)	$1.51 \cdot 10^{-2}$ (T; Ref. 7)	$1.3 \cdot 10^{-2}$
394.3	1034 (Ref. 7)	$2.30 \cdot 10^{-2}$ (T; Ref. 7)	$2.0 \cdot 10^{-2}$
400.4	1379 (Ref. 7)	$2.72 \cdot 10^{-2}$ (T; Ref. 7)	$2.4 \cdot 10^{-2}$
417.6	1724 (Ref. 7)	$4.21 \cdot 10^{-2}$ (T; Ref. 7)	$3.9 \cdot 10^{-2}$
422.0	2068 (Ref. 7)	$4.74 \cdot 10^{-2}$ (T; Ref. 7)	$4.5 \cdot 10^{-2}$
423.2	1254.8 (Ref. 35)	$3.11 \cdot 10^{-2}$ (D; Ref. 35)	$4.6 \cdot 10^{-2}$
431.5	2413 (Ref. 7)	$5.75 \cdot 10^{-2}$ (T; Ref. 7)	$5.8 \cdot 10^{-2}$
442.6	2758 (Ref. 7)	$7.30 \cdot 10^{-2}$ (T; Ref. 7)	$7.8 \cdot 10^{-2}$
449.8	290 (Ref. 7)	$8.44 \cdot 10^{-2}$ (T; Ref. 7)	$9.3 \cdot 10^{-2}$
452.6	600 (Ref. 7)	$9.02 \cdot 10^{-2}$ (T; Ref. 7)	$1.0 \cdot 10^{-1}$
460.4	1158 (Ref. 7)	$1.032 \cdot 10^{-1}$ (T; Ref. 7)	$1.2 \cdot 10^{-1}$
468.2	1972 (Ref. 7)	$1.294 \cdot 10^{-1}$ (T; Ref. 7)	$1.5 \cdot 10^{-1}$
473.2	3516 (Ref. 35)	$1.10 \cdot 10^{-1}$ (D; Ref. 35)	$1.7 \cdot 10^{-1}$
477.6	3241 (Ref. 7)	$1.403 \cdot 10^{-1}$ (T; Ref. 7)	$1.9 \cdot 10^{-1}$

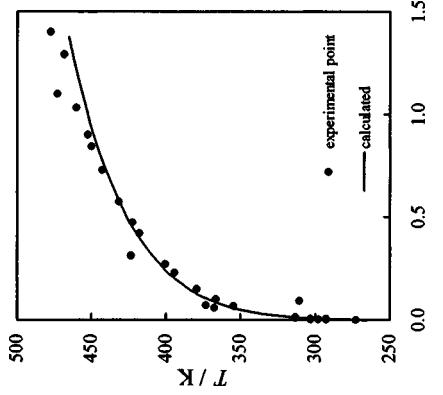


Fig. 5. All the solubility data for water (2) in hexane (1).

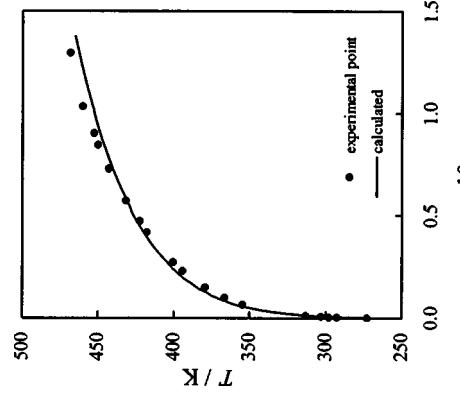


Fig. 6. Recommended and tentative solubility data for water (2) in hexane (1).

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szlegla⁴² are independent data. These data are therefore Rejected. The data reported by Booth and Everson,⁵ Bennet and Philip,³⁷ Gester,³⁸ Gill et al.,³⁹ Hicks and Young,⁴¹ Milligan,⁴³ Rasilov,⁴⁴ Roof,⁴⁵ Scott and van Konynenburg,⁴⁷ lack sufficient information to justify evaluation. Therefore these data are Rejected. The publications of Herz⁴⁰ and Scheffer⁴⁶ were not accessible for compilers.

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Components:	Original Measurements:			
(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	G. Barone, V. Crescenzi, B. Pispisa, and P. Quandriglio, J. Macromol. Chem. 1 , 761 (1966).	(1) Hexane; C ₆ H ₁₄ ; [110-54-3]		
(2) Water; H ₂ O; [7732-18-5]		(2) Water; H ₂ O; [7732-18-5]		
Prepared By:		Prepared By:		
Variables:	One temperature: 25 °C			
One temperature: 303 K	A. Maczynski			
Experimental Data				
The authors report a value of 9.6·10 ⁻⁴ mol(1)/L(2) for the solubility of hexane in water at 25 °C. This value is the experimental one multiplied by 760/P where P is the partial pressure of (1) over (2), P = 149 mm Hg. The solubility at system pressure calculated by the compiler is 1.882·10 ⁻⁴ mol(1)/L(2) and the corresponding mass percent and mole fraction, x ₁ , are 0.001621 g(1)/100 g sln and 3.385·10 ⁻⁶ .	The solubility of water in hexane at 303 K was reported to be 0.0051 g(2)/100 g sln. The corresponding mole fraction, x ₂ , value calculated by compiler is 0.00024.			
Auxiliary Information				
Method/Apparatus/Procedure:	Source and Purify of Materials:			
The saturation was carried out by bubbling the vaporized (1) into the solution and letting an excess of the condensed (1) stand in contact with the aqueous phase for more than 12 h at 25 °C under gentle shaking. 0.20 mL samples of (2) saturated with (1) were taken with a calibrated syringe and injected into the chromatographic column packed with 1.5% of poly(propylene glycol) on chromosorb. A gas chromatography unit having a tungsten wire kathometer as detector was employed. More details are given in the paper.	(1) Source not specified; purified; purity not specified. (2) Distilled.			
Estimated Error:				
Not specified.				
Method/Apparatus/Procedure:	Source and Purify of Materials:			
Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.	(1) RP product, C. Erba, Milan; chromatographically pure. (2) Not specified.			
Estimated Error:				
Temperature: ±0.02 °C. Solubility: ±4% (type of error not specified).				
References:				
J. Timmermans, <i>Physico-Chemical Constants of Pure Organic Compounds</i> (Elsevier, New York, 1950).				

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	L. S. Budaniseva, T. M. Lesieva, and M. S. Nemtsov, Zh. Fiz. Khim. 50 , 1344 (1976).	
Variables:	Components:	
One temperature: 20 °C	(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	L. S. Budaniseva, T. M. Lesieva, and M. S. Nemtsov, Zh. Fiz. Khim. 50 , 1344 (1976).
Prepared By:	Prepared By:	
A. Maczynski	A. Maczynski	
Experimental Data	Experimental Data	
The solubility of hexane in water at 20 °C was reported to be $x_1 = 3 \cdot 10^{-6}$. The corresponding mass percent calculated by the compiler is 0.0014 g(1)/100 g sln. The solubility of water in hexane at 20 °C was reported to be $x_2 = 3.7 \cdot 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.0077 g(2)/100 g sln.	<p>The solubility of hexane in water at 20 °C was reported to be $x_1 = 3 \cdot 10^{-6}$. The corresponding mass percent calculated by the compiler is 0.0014 g(1)/100 g sln. The solubility of water in hexane at 20 °C was reported to be $x_2 = 3.7 \cdot 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.0077 g(2)/100 g sln.</p>	
Auxiliary Information	Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:	
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) Source not specified; pure or analytical reagent grade; purity <99.9%. (2) Not specified.	(1) Source not specified; pure or analytical reagent grade; purity <99.9%. (2) Not specified.
Estimated Error:	Estimated Error:	
Not specified.	Not specified.	

Original Measurements:		Components:		Original Measurements:	
Components:		(1) Hexane; C_6H_{14} ; [110-54-3]		A. K. Charykov, V. I. Tikhomirov, and T. M. Potapova, Zh. Obshch. Khim. 48 , 1916 (1978).	
(1) Hexane; C_6H_{14} ; [110-54-3]		(2) Water; H_2O ; [7732-18-5]			
Variables:		Prepared By:		Prepared By:	
Temperature and Pressure		M. C. Haulait-Pirson		M. C. Haulait-Pirson	
Experimental Data					
Hydrocarbon-rich liquid phase composition for the three-phase conditions					
$t/^\circ F$	T/K (compiler)	x_2 (compiler)	$g(2)/100\text{ g sln}$	P/psia	P/MPa (compiler)
179	354.82	0.0067	0.14	30	0.207
223	379.26	0.0151	0.32	60	0.414
261	400.37	0.0272	0.58	100	0.689
292	417.59	0.0421	0.91	150	1.034
317	431.48	0.0575	1.26	200	1.379
337	442.59	0.0730	1.62	250	1.724
355	452.59	0.0902	2.03	300	2.068
369	460.37	0.1032	2.35	350	2.413
383	468.15	0.1294	2.78	400	2.758
200	366.48	0.0100	0.21	42	0.290
250	394.26	0.0230	0.49	87	0.600
300	422.04	0.0474	1.03	165	1.138
350	449.82	0.0844	1.89	286	1.972
400	477.50	0.1403	3.30	470	3.241
Auxiliary Information					
Method/Apparatus/Procedure:					
The vapor and liquid phase compositions have been determined for the (1)- $\text{--}(2)$ system in the two-phase hydrocarbon-rich liquid region. Equilibrium points were obtained by incremental addition of water followed by stirring, settling, sampling, and chromatographic analysis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. Many details are given in the paper.					
Source and Purity of Materials:					
(1) Phillips Petroleum Company; 99.5% purity. (2) Laboratory distilled.					
Estimated Error:					
Solubility: ± 0.004 weight fraction of the (2) present.					

Components:	Original Measurements:		
(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	Th. W. De Loos, W. G. Penders, and R. N. Lichtenhauer, J. Chem. Thermodyn. 14, 83 (1982).		
(2) Water, H ₂ O; [7732-18-5]	632.0 634.9 637.7 639.3 641.1 641.6 641.8 641.9 641.3 641.2 640.8 637.4 635.4 635.8 635.9 635.9 637.7 637.7 639.3 641.1 641.4 643.5 644.2 644.8 645.3 645.5 645.4 645.4 645.3 644.2 643.3 643.3 642.1 642.1 641.2 640.0 640.0 639.7 639.7 634.6 634.6 632.4 628.4 625.1 623.1 620.7 618.3 616.4 614.8 613.4 610.9 609.5 608.4 607.5 606.3 605.1 604.2 603.2 601.8 600.4 597.6 596.7 596.3 595.9 595.9 629.9		
Variables:	Prepared By: C. L. Young		
Temperature, pressure	Values of pressure and temperature on one phase-two phase boundary		
	Experimental Data		
T/K	x ₁	g(1)/100 g sln	P/MPa
631.5	0.005	2.4	18.33
633.8			18.82
635.9			19.31
637.7			19.80
639.7			19.80
641.4			20.27
643.5			20.76
644.2			21.25
644.8			21.74
645.3			22.08
645.5			22.08
645.4			22.20
645.4			22.22
644.2			22.23
643.3			22.23
643.3			22.18
642.1			22.18
642.1			22.08
641.2			21.99
640.0			21.89
640.0			21.78
639.7			21.35
639.7			21.13
634.6			21.13
634.6			20.73
632.4			20.34
628.4			19.97
625.1			19.63
623.1			19.37
620.7			19.37
618.3			19.23
616.4			19.15
614.8			19.10
613.4			19.10
610.9			19.20
609.5			19.20
608.4			19.25
607.5			19.40
606.3			19.45
605.1			19.66
604.2			19.80
603.2			20.00
601.8			20.30
600.4			20.63
597.6			21.92
596.7			22.41
596.3			24.69
595.9			26.23
595.9			26.58
629.9	0.015	6.8	18.33
			635.0

24.79	630.5	23.13
24.90	630.1	23.48
25.05	632.4	24.01
25.15	631.9	24.22
25.38	631.5	24.31
25.63	631.3	24.41
25.77	631.2	24.46
26.02	631.1	24.51
26.41	631.0	24.55
27.22	630.8	24.62
28.32	630.0	24.95
29.62	628.6	25.82
30.60	627.8	26.50
31.57	627.5	26.92
32.07	627.3	27.27
32.80	627.1	27.65
34.50	626.8	28.15
35.47	626.7	28.63
36.50	626.6	29.12
36.84	626.6	30.10
37.93	626.7	31.09
40.18	626.9	32.07
42.38	627.2	33.54
45.08	628.8	36.94
57.56	629.2	38.31
60.75	631.4	42.63
69.54	633.7	47.53
78.36	639.1	57.23
79.35	643.9	664.0
86.68	648.7	641.2
102.87	655.9	643.2
17.61	659.8	648.3
18.11	664.4	648.3
18.35	671.2	648.3
18.84	616.3	643.2
20.56	618.3	643.2
20.78	622.3	648.3
21.27	623.4	648.3
21.51	626.6	648.3
21.76	628.4	648.3
22.25	629.9	648.3
22.74	631.4	648.3
24.55	633.8	648.3
24.95	633.5	648.3
25.29	633.2	648.1
26.26	632.6	647.9
28.83	632.3	647.8
29.42	632.0	647.7
30.42	631.0	647.7

627.6	30.89	627.6	22.27
627.7	31.57	628.3	23.23
627.8	32.86	628.3	24.22
628.1	33.52	628.2	25.19
628.3	34.50	628.0	25.70
628.7	36.94	629.0	34.50
629.7	40.18	629.7	35.47
631.5	47.05	630.1	36.94
635.0	56.82	631.0	38.41
641.9	68.33	632.1	40.18
647.7	78.63	632.3	40.67
653.5	91.45	632.8	41.40
660.1	98.94	633.1	41.90
663.9	24.31	633.5	42.63
618.9	633.8	633.8	43.12
619.3	18.25	634.3	43.85
620.1	18.35	645.0	60.26
621.0	18.59	647.2	64.66
622.5	19.33	650.1	69.54
626.1	20.70	654.5	76.79
629.2	21.34	657.9	83.02
628.9	22.15	662.7	92.08
628.6	22.74	665.4	98.94
629.3	23.53	671.2	108.75
629.4	24.12	671.7	109.98
629.2	24.54	608.9	16.65
628.9	25.00	612.1	17.47
628.6	25.52	615.0	18.37
629.4	26.18	618.3	19.33
627.9	27.17	619.5	19.77
627.5	18.25	621.1	20.31
627.3	18.35	621.5	20.55
627.2	18.59	622.1	20.80
627.3	18.84	622.8	21.29
627.5	28.15	623.8	21.78
627.3	29.12	624.6	22.27
627.2	30.10	625.6	23.25
627.3	31.09	626.0	24.72
627.5	31.07	626.1	25.70
627.8	33.05	626.3	27.17
628.0	34.00	626.6	29.62
628.3	34.99	627.0	31.09
628.7	34.50	627.6	32.56
628.6	36.68	628.1	33.54
631.6	40.18	628.5	34.50
634.4	45.08	59.79	37.93
643.7	644.4	630.5	37.93
652.9	74.44	633.3	42.63
660.7	660.7	634.8	45.08
616.3	17.78	637.8	49.98
631.6	18.13	641.0	54.87
617.3	18.40	644.4	59.72
619.0	19.33	645.9	62.22
621.3	19.82	647.1	64.68
622.8	20.31	653.3	74.44
624.0	20.80	660.1	86.68
625.2	21.29	667.9	101.40
626.1	21.78	673.9	111.20

0.102	17.98	648.6	67.09
613.4	18.03	652.7	74.44
613.8	18.37	656.8	81.79
614.5	18.61	662.3	91.59
615.2	18.86	667.2	101.40
616.1	19.25	672.1	111.20
617.4	19.82	608.3	42.7
618.7	20.31	609.1	0.135
619.8	20.80	609.8	
621.1	21.29	611.3	
622.0	22.27	615.0	18.86
623.4	22.96	616.0	20.33
624.1	23.74	616.8	20.82
624.9	24.72	617.7	18.13
625.3	25.94	618.4	18.37
625.6	27.17	619.1	
625.9	28.63	620.3	
626.4	30.10	621.0	
626.7	31.09	622.2	
627.1	32.97	622.9	
627.5	33.05	623.4	
627.9	34.50	624.1	
628.9	36.94	624.9	
630.0	41.40	625.8	
632.8	59.77	627.3	
643.9	74.44	628.2	
652.9	74.44	629.4	
653.1	75.67	631.2	
653.5	76.90	632.7	
654.2	86.68	634.2	
660.0	98.94	635.9	
666.6	18.08	643.7	
610.2	19.10	647.0	
613.1	19.84	653.1	
614.2	21.12	659.9	
617.7	21.78	666.5	
618.7	23.01	672.6	
620.5	23.74		
621.4	24.48		
622.1	25.21		
622.6	26.18		
623.2	27.17		
623.6	28.15		
624.2	29.12		
624.6	30.10		
625.1	31.09		
625.7	32.97		
626.2	33.54		
627.0	34.52		
627.6	35.47		
628.3	37.43		
628.4	40.18		
631.3	42.63		
632.9	46.35		
635.4	49.98		
637.7	57.32		
642.5	62.22		
645.6			

Auxiliary Information

Source and Purity of Materials:

- (1) Merck sample, purity at least 99.0 mole % degassed.
 (2) Doubly distilled; conductivity less than 10^{-6} S/cm.

Estimated Error:

- Temperature: $\delta T/K = \pm 0.1$ K.
 Pressure: $\delta P/MPa = \pm 0.02$ up to 40 MPa, ± 0.05 above 40 MPa.
 Solubility: $\delta x = \pm 0.002$.

References:

- [1] Th. W. De Loos, A. J. M. Wijen, and G. A. M. Dipen, *J. Chem. Thermodyn.*, **12**, 193 (1980).

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugulukov, and M. A. Pyranishnikova, Khim. Tekhnol. Topl. Mysel 10 , 42 (1965).
Prepared By:	Prepared By:	
M. C. Haulait-Pirson	A. Maczynski and M. C. Haulait-Pirson	
Variables:	Variables:	
One temperature: 16 °C	Temperature: 20 °C–40 °C	
Experimental Data	Experimental Data	
The solubility of hexane in water at 16 °C was reported to be 0.055 mL(1)/L(2). With the assumption of a solution density of 1.00 g./mL and a density value of 0.6629 g./mL for hexane at 16 °C (Timmermans ²), the corresponding mass percent is 0.0036 g(1)/100 g sln and the corresponding mole fraction, x ₁ , is 7.5·10 ⁻⁶ (compiler).	Solubility of water in hexane	
Auxiliary Information	Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:	
The thermostatic method described in Durand ¹ was used. Addition of pipeted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.	(1) Not specified. (2) Distilled.	20 30 40
Estimated Error:	Solubility: ± 0.005 mL(1)/L(2).	
References:	¹ R. Durand, C. R. Hebd. Seances Acad. Sci., 226 , 409 (1948). ² J. Timmermans, <i>Physico-Chemical Constants of Pure Organic Compounds</i> (Elsevier, New York, 1950).	
Method/Apparatus/Procedure:	Source and Purity of Materials:	
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was determined.	(1) Not specified. (2) Not specified.	0.0101 0.0179 0.0317
Estimated Error:	Not specified.	

Components:		Original Measurements:		Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	H. Föhner, Ber. Dtsch. Chem. Ges. 57 , 510 (1924).	(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	J. H. Jones and J. F. McCants, Ind. Eng. Chem. 46 , 1956 (1954).	(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	J. H. Jones and J. F. McCants, Ind. Eng. Chem. 46 , 1956 (1954).
(2) Water; H ₂ O; [7732-18-5]		(2) Water; H ₂ O; [7732-18-5]		(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:	Prepared By:	Prepared By:	Variables:	Prepared By:
One temperature: 15.5 °C	M. C. Haulait-Pirson	M. C. Haulait-Pirson	M. C. Haulait-Pirson	One temperature: 100 °F	M. C. Haulait-Pirson
Experimental Data		Experimental Data		Experimental Data	
The solubility of hexane in water at 15.5 °C was reported to be 0.022 mL(1)/100 mL sln or 0.014 g(1)/100 g sln.	The corresponding mole fraction, x_1 , calculated by the compiler is $2.92 \cdot 10^{-5}$.	The solubility of hexane in water at 100 °F (37.78 °C) was reported to be 0.4 g(1)/100 g sln.	The corresponding mole fraction, x_1 , calculated by the compiler is $8.3 \cdot 10^{-4}$.	The solubility of water in hexane at 100 °F (37.78 °C) was reported to be 0.2 g(1)/100 g sln.	The solubility of water in hexane at 100 °F (37.78 °C) was reported to be 0.2 g(1)/100 g sln.
				The corresponding mole fraction, x_2 , calculated by the compiler is $9.5 \cdot 10^{-3}$.	
Auxiliary Information		Auxiliary Information		Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purify of Materials:	Method/Apparatus/Procedure:	Source and Purify of Materials:	Method/Apparatus/Procedure:	Source and Purify of Materials:
In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 mL of (2) until a completely clear solution was obtained at the experimental temperature.	(1) Source not specified; commercial grade; used as received. (2) Not specified.	The solubility of (2) in (1) was obtained by titrating (1), brought to 100 °F. As the cloud point was approached, (2) was added dropwise and the flask agitated in the 100 °F constant temperature bath. The solubility of (1) in (2) was determined by titrating (2) at 100 °F with (1).	(1) Phillips; used as received; n_D^{20} 1.3745, d_4^{25} 0.6607. (2) Distilled; n_D^{20} 1.3350.	(1) Phillips; used as received; n_D^{20} 1.3745, d_4^{25} 0.6607. (2) Distilled; n_D^{20} 1.3350.	(1) Phillips; used as received; n_D^{20} 1.3745, d_4^{25} 0.6607. (2) Distilled; n_D^{20} 1.3350.
Estimated Error:	Not specified.	Estimated Error:	Not specified.	Estimated Error:	Temperature: ± 0.2 °F.

Components:	Original Measurements:	Original Measurements:
(1) Hexane; C_6H_{14} ; [110-54-3] (2) Water; H_2O ; [7732-18-5]	J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib., 9, 279 (1982).	I. M. Korenman and R. P. Arefeva, Patent USSR, 553 524, 5 April 1977.
Prepared By:	Prepared By:	Prepared By:
G. T. Heffter	A. Maczynski	A. Maczynski
Variables:	Variables:	Variables:
Temperature: 15 °C–35 °C	One temperature: 20 °C	One temperature: 20 °C
Experimental Data	Experimental Data	Experimental Data
Solubility of hexane in water	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot g(1)/100 \text{ g sln}$ (compiler)
		$\text{mg}(1)/\text{kg}(2)$
15	2.24	1.07
20	2.15	1.03
25	2.11	1.01
30	2.09	1.00
35	2.11	1.01
Auxiliary Information	Source and Purity of Materials:	Method/Apparatus/Procedure:
	(1) Not specified. (2) Not specified.	About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg. of an insoluble indicator was added and (1) was microbureted until the indicator floated to form a colored thin layer on the cylinder wall 2–3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5–1.5 min.
	Estimated Error:	Not specified.

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) 51, 937 (1978).	
Variables:	Prepared By:	
One temperature: 25 °C	A. Maczynski and Z. Maczynska	
Experimental Data		Source and Purify of Materials:
The solubility of hexane in water at 25 °C was reported to be 0.16 g(1)/L sln. The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.016 g(1)/100 g sln and $3.3 \cdot 10^{-5}$. The compiler's calculations assume a solution density of 1.00 g/ml.		(1) Source not specified; CP reagent; purity not specified. (2) Distilled.
Auxiliary Information		Method/Apparatus/Procedure:
		A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom stoppered vessel and vigorously stirred magnetically for 10–12 h. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.
Method/Apparatus/Procedure:		Source and Purify of Materials:
About 200–500 mL (2) was placed in a ground-joint glass cylinder and 20–50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer. Blanks were made to determine the excess of (1).		(1) Not specified. (2) not specified.
Estimated Error:		Estimated Error:
Solubility: 0.01 g(1)/L sln (standard deviation from 6 determinations).		Solubility: 0.01 g(1)/L sln (standard deviation from 6 determinations).

Auxiliary Information

Components:
 (1) Hexane; C₆H₁₄; [110-54-3]
 (2) Water; H₂O; [7732-18-5]

Variables:
 Temperature: 100 °F–280 °F
 Pressure: 24 psia–525 psia

Method/Apparatus/Procedure:
 Apparatus for producing equilibrium conditions and analytical procedure are the same as described in Davis.¹ No more details are given in the paper.

Source and Purity of Materials:
 (1) Phillips Petroleum Co.; certified purity of at least 99.0 mole %; used as received.
 (2) Distilled; boiled to remove any dissolved gases.

Estimated Error:
 Not specified.

References:
 J. E. Davis, M. S. Thesis, The University of Texas, Austin, 1959.

Experimental Data
Solubility of hexane in water

t/°F	T/K	10 ⁴ ·x ₁	g(1)/100 g sln (compiler)	P/psia	P/MPa (compiler)
100	310.94	0.2214	0.01060	24.8	0.171
		0.302	0.01446	41.2	0.284
		0.319	0.01527	74.9	0.516
		0.342	0.01637	101.1	0.697
		0.359	0.01623	133.8	0.923
		0.342	0.01637	220.2	1.518
		0.3398	0.01627	308.5	2.127
		0.3396	0.01626	422.5	2.913
		0.342	0.01637	513.0	3.537
		0.398	0.01905	45.2	0.312
160	344.27	0.541	0.02590	75.3	0.519
		0.644	0.03083	112.6	0.776
		0.6349	0.03039	172.2	1.187
		0.633	0.03030	252.0	1.737
		0.64	0.03063	338.6	2.335
		0.648	0.03102	432.2	2.980
		0.64	0.03063	488.1	3.365
		0.6349	0.01886	80.3	0.554
		0.608	0.02910	116.6	0.804
		0.87	0.04164	174.8	1.205
220	377.60	1.08	0.05169	233.3	1.609
		1.08	0.05169	233.3	1.609
		1.092	0.05226	282.5	1.948
		1.112	0.05322	355.1	2.448
		1.09	0.05217	444.4	3.064
		1.11	0.05312	524.8	3.618
		0.272	0.01302	98.2	0.677
		0.475	0.02274	137.5	0.948
		0.826	0.03953	205.0	1.413
		1.155	0.05527	268.8	1.853
280	410.94	1.478	0.07072	353.9	2.440
		1.588	0.07598	392.2	2.704
		1.685	0.08062	455.0	2.999
		1.772	0.08478	506.5	3.492

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. 51 , 230 (1973).	J. Liu, Z. Qin, and J. Wang, J. Chem. Eng. Data 47 , 1243 (2002).
Prepared By:	Prepared By:	
M. C. Haulait-Pirson	A. Skrzecz and B. Wisniewska-Gocłowska	
Variables:	Variables:	
One temperature: 25 °C	Temperature: 298.15 K–318.15 K	
Experimental Data	Experimental Data	
The solubility of hexane in water at 25 °C was reported to be 12.5 mg(1)/L sln corresponding to a mole fraction, x_1 , of $2.5 \cdot 10^{-6}$. The corresponding mass percent calculated by the compiler is 0.00123 g(1)/100 g sln. The compiler's calculation assumes a solution density of 1.00 g/mL.	Solubility of water in hexane	
	<i>T/K</i>	<i>x₁</i>
	298.15	0.377
	308.15	0.369
	318.15	0.360
Auxiliary Information	Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:	
A mixture of (1) and (2) was equilibrated for at least 12 h in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 h and the aqueous phase was tested (Tyndall effect). Both phases were analyzed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by glc. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.	(1) Phillips Petroleum Co.; research grade; purity 99+%; used without further purification. (2) Doubly distilled.	(1) Tianjin Tian-Da Chemical Factory; purity >97.0%; passed through columns containing silica gel and basic alumina; purity >99.5 mole % by glc. (2) Deionized and distilled.
Estimated Error:	Estimated Error:	
Temperature: ± 0.1 °C. Solubility: ± 1 mg(1)/L sln.	Temperature: ± 0.05 K.	

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. 573, 251 (1975).	
Variables:	Components:	
Not specified	(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).
Prepared By:	Original Measurements:	
M. C. Haulait-Pirson	C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
Experimental Data	Experimental Data	
The authors reported the value of 16.2 mg(1)/L sln for the solubility of hexane in water. With the assumption of a solution density of 1.00 g./mL, the corresponding mass percent, calculated by the compiler, is 0.00162 g(1)/100 g sln and the corresponding mole fraction, x_1 , is $3.4 \cdot 10^{-6}$.	The solubility of hexane in water at 25 °C was reported to be 9.5 mg(1)/kg sln (0.00095 g(1)/100 g sln). The corresponding mole fraction, x_1 , calculated by the compiler is $1.99 \cdot 10^{-6}$. The same value is also reported in McAuliffe. ^{1,2}	
Auxiliary Information	Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purify of Materials:	
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μ L sample of (1) saturated water was withdrawn with a Hamilton Syringe and injected into the Fractionator of a gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	(1) Phillips Petroleum Co.; 99+ % purity; used as received. (2) Distilled.	
(1) was partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to a column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibration it was possible to calculate the amount of (1) in the original sample.	Estimated Error: Temperature: ± 1.5 °C. Solubility: 1.3 mg(1)/kg sln (std. dev. of mean),	
	References:	
	I.C. McAuliffe, Nature (London) 200 , 1092 (1963). C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. 9 , 275 (1964),	

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	J. W. McBain and K. J. Lissant, J. Phys. Colloid Chem., 55 , 665 (1951).	
Prepared By:		
Variables:		
One temperature: 25 °C	Variables:	One temperature: 100 °F (311 K)
Experimental Data		
The solubility of hexane in water at 25 °C was reported to be 0.012 g(1)/100 mL sln. With the assumption of a solution density of 1.00 g./mL, the corresponding mass percent is 0.012 g(1)/100 g sln and the corresponding mole fraction, x_1 , is $2.5 \cdot 10^{-5}$ (compiler).		
Auxiliary Information		
Method/Apparatus/Procedure:	Source and Purity of Materials:	
10 mL of (2) was pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the solubility.	(1) C.P. grade. (2) Distilled and boiled to remove CO ₂ .	
Estimated Error:		
Not specified.		
References:		
E. R. Washburn, V. Hnizda, and R. D. Vold, J. Am. Chem. Soc., 53 , 3232 (1931).		

Components:	Original Measurements:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. 45 , 454 (1953).	
Prepared By:		
Variables:		
One temperature: 100 °F (311 K)	Variables:	One temperature: 100 °F (311 K)
Experimental Data		
The solubility of hexane in water at 100 °F (311 K) was reported to be <0.1 g(1)/100 g sln. The corresponding mole fraction, x_1 , calculated by the compiler, is $<2 \cdot 10^{-4}$. The solubility of water in hexane at 100 °F (311 K) was reported to be <0.1 g(2)/100 g sln. The corresponding mole fraction, x_2 , calculated by the compiler, is $<5 \cdot 10^{-3}$.		
Auxiliary Information		
Method/Apparatus/Procedure:	Source and Purity of Materials:	
The method was essentially that of Washburn <i>et al.</i> ¹ and involved titration of the second component to the cloud point, in a constant temperature bath.	(1) Phillips; pure grade; used without further purification; n_D^{20} 1.3752. (2) Distilled.	
Estimated Error:		
Not specified.		
References:		
E. R. Washburn, V. Hnizda, and R. D. Vold, J. Am. Chem. Soc., 53 , 3232 (1931).		

Components:		Original Measurements:		Original Measurements:	
(1) Hexane; C_6H_{14} ; [110-54-3]	A. Yu. Namiot, V. G. Skripka, and Yu. G. Lotter, <i>Zh. Fiz. Khim.</i> 50 , 2718 (1976); Deposited doc. VINITI 1213-76.	(1) Hexane; C_6H_{14} ; [110-54-3]	H. D. Nelson and C. L. De Ligny, <i>Rec. Trav. Chim. Pay-Bas Belg.</i> 87 , 528 (1968).	(2) Water; H_2O ; [7732-18-5]	
(2) Water; H_2O ; [7732-18-5]		(2) Water; H_2O ; [7732-18-5]			
Prepared By:		Prepared By:		Prepared By:	
Variables:		Temperature: 4 °C–35 °C		M. C. Haulair-Prison	
Temperature: 200 °C and 220 °C		Experimental Data		Experimental Data	
Pressure: 2.0 MPa–5.2 MPa		Solubility of water in hexane		Solubility of hexane in water	
Experimental Data		Experimental Data		Experimental Data	
Solubility of water in hexane		Solubility of hexane in water		Solubility of hexane in water	
$t/^\circ\text{C}$		x_2		$t/^\circ\text{C}$	
$t/^\circ\text{C}$		$g(2)/100 \text{ g sln}$ (compiler)		$10^6 \cdot x_1$	
$t/^\circ\text{C}$		$P/\text{kg} \cdot \text{cm}^{-2}$		$\text{mg}(1)/\text{kg sln}$ (compiler)	
200		0.006		3.42 ± 0.34	
200		0.024		3.17 ± 0.52	
200		0.051		3.83 ± 0.47	
200		0.084		2.69 ± 0.26	
200		0.097		4.64 ± 0.72	
220		0.002		2.22	
220		0.023		4.42 ± 0.26	
220		0.053		21.2	
220		0.088			
220		0.129			
220		0.179			
220		0.216			
Method/Apparatus/Procedure:		Source and Purity of Materials:		Source and Purity of Materials:	
The static method for vapor–liquid equilibrium described in Sultany <i>et al.</i> ¹ was used. No more details were reported in the paper.		(1) Fluka purum.		(1) Fluka purum.	
		(2) Tap-water was refluxed for 8 hours in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.		(2) Tap-water was refluxed for 8 hours in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.	
Estimated Error:		Estimated Error:		Estimated Error:	
		Solubility: error given above (90% probability interval).		Solubility: error given above (90% probability interval).	
Method/Apparatus/Procedure:		Source and Purity of Materials:		Source and Purity of Materials:	
The static method for vapor–liquid equilibrium described in Sultany <i>et al.</i> ¹ was used. No more details were reported in the paper.		(1) Source not specified; CP reagent; used as received.		(1) Source not specified; CP reagent; used as received.	
		(2) Distilled.		(2) Distilled.	
Estimated Error:		Estimated Error:		Estimated Error:	
Not specified.		Not specified.		Not specified.	
References:		References:		References:	
		¹ R. G. Sultanov, V. E. Skripka, and Yu. A. Namiot, <i>Zh. Fiz. Khim.</i> 46 , 2170 (1976).			

Components:		Original Measurements:		Original Measurements:	
		J. Polak and B. C.-Y. Lu, Can. J. Chem., 51 , 4018 (1973).		L. C. Price, Am. Assoc. Pet. Geol. Bull., 60 , 213 (1976).	
(1) Hexane; C_6H_{14} ; [110-54-3]		(1) Hexane; C_6H_{14} ; [110-54-3]		(1) Hexane; C_6H_{14} ; [110-54-3]	
(2) Water; H_2O ; [7732-18-5]		(2) Water; H_2O ; [7732-18-5]		(2) Water; H_2O ; [7732-18-5]	
Variables:		Prepared By:		Prepared By:	
Temperature: 0 °C–25 °C		M. C. Haulait-Pirson		F. Kapuku	
Experimental Data		Experimental Data		Experimental Data	
Solubility of hexane in water		Solubility of hexane in water at system pressure		Solubility of hexane in water at system pressure	
$t/^\circ\text{C}$		$10^6 \cdot x_1$ (compiler)		$10^6 \cdot x_1$ (compiler)	
0 ^a		mg(1)/kg sln		g(1)/100 g sin (compiler)	
25 ^b		16.5 ^c		0.000947	
		2.59		9.47±0.20	
		12.4 ^c		10.1±0.3	
		55.7		13.2±0.5	
		69.7		15.4±1.9	
		69.7		15.2±0.5	
		99.1		10.0±0.10	
		114.4		0.00132	
		121.3		0.00154	
		137.3		0.00152	
		151.8		0.00224	
		11.89		0.00292	
		22.2		37.6±1.2	
		106.0±4.0		56.9±2.3	
		0.0106		0.0106	

^{a–e}See Estimated Error.

Auxiliary Information

Source and Purity of Materials:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

Source and Purity of Materials:

Room-temperature solubility was determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of a gas chromatograph. The solutions were prepared in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to a gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:

Temperature: (a) ±0.02 °C; (b) ±0.01 °C.
Solubility: (c) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).

Estimated Error:

Temperature: ± 1 °C.
Solubility: range of values given above.

Components:	Original Measurements:					
(1) Hexane; C ₆ H ₁₄ ; [110-54-3]	C. J. Rebert and K. E. Hayworth, AIChE J. 13 , 118 (1967).					
(2) Water; H ₂ O; [7732-18-5]	22.5 23.0 23.5 24.0 24.5 25.0 25.5 26.0 26.5 27.0 27.5 28.0 28.5 19.53 21.63 4.63 5.06 5.52 6.01 6.53 6.97 7.74 8.49 9.31 10.23 11.34 12.92 14.88 14.88 17.39					
Variables:	Prepared By:					
Pressure and temperature on one phase-two phase boundary	C. L. Young					
Experimental Data						
Smoothed data						
<i>t</i> /°C	<i>T</i> /K	<i>x</i> ₁	<i>g</i> (1)/100 g sin			
330	603	0.0042	2.0			
340	613					
350	623					
360	633					
370	643					
371	644					
371.8	645.0 ^a					
371	644 ^a					
370	643					
360	633					
350	623					
340	613					
335	608					
332	605					
330	603					
328	601					
326	599					
324	597					
322	595					
318	591					
315	588					
300	573					
310	583					
320	593					
325	598					
330	603					
335	608					
340	613					
345	618					
350	623					
355	628					
360	633					
270	543		0.1762			
275	548					
280	553					
285	558					
290	563					
295	568					
300	573					
305	578					
310	583					
315	588					
320	593					
325	598					

Auxiliary Information**Source and Purity of Materials:**

(1) No details given.

Estimated Error:Temperature: δT /K = ± 0.05 .
Solubility: δP /MPa = ± 0.007 .**References:**C. J. Rebert and W. B. Kay, AIChE J. **5**, 285 (1959).

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Original Measurements:	
J. W. Roddy and C. F. Coleman, Talanta 15, 1281 (1968).	V.G. Skripka, Tr. Vses. Neftegazov. Nauch.-Issled. Inst. 61, 139 (1976), R. G. Sultanov and V. G. Skripka, Zh. Fiz. Khim. 47, 1035 (1973); Deposited doc. 1976, VINITI 5347-72.
Prepared By:	
M.C. Haufler-Pinson	
Experimental Data	
Variables:	Temperature: 200 °C and 220 °C Pressure: 3.6 MPa–78.5 MPa
Experimental Data	
One temperature: 25 °C	The solubility of water in hexane at 25 °C was reported to be 0.00362 mol(2)/L sln corresponding to a mole fraction, x_2 , of $4.76 \cdot 10^{-4}$. The corresponding mass percent value calculated by the compiler is 0.00995 g(2)/100 g sln. The compiler's calculation assumes a solution density of 0.6629 g/mL (the density of hexane reported in Timmermans ¹⁾ .
Auxiliary Information	
Source and Purity of Materials:	(1) Phillips Petroleum Co.; 99%; purified by shaking with concentrated sulfuric acid, washed with water and dried with sodium sulfate. (2) Tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/mL.
Method/Apparatus/Procedure:	A method of gravimetric absorption monitored by tritium tracer was used. (1) was equilibrated with a slight excess of deionized water by shaking over a period of at least 8 h in a thermostatic bath. The phases were allowed to separate for at least 16 h and then were sampled for tritium analysis. Most of the (1) phase was weighed into a boiling flask of a closed distillation system and then distilled through a magnesium perchlorate weighing tube. The magnesium perchlorate was then dissolved for measurement of its tritium content with a Packard Tri-Carb Scintillation Spectrometer.
Estimated Error:	Solubility: better than 1% (type of error not specified).
References:	J. Timmermans, <i>Physico-Chemical Constants of Pure Organic Compounds</i> (Elsevier, New York, 1950).

Auxiliary Information

Source and Purity of Materials:

The experimental technique was described in Sultanov *et al.*¹. No details reported in the paper.

- (1) Source not specified, chemical reagent grade; purity not received.
- (2) Distilled.

Estimated Error:

References:
I.R. G. Sulitanov, V. E. Skripka, and Yu. A. Namiot, *Gazov. Prom.* **4**, 6 (1971).

Components:	Original Measurements:		
(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]	(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]		
Prepared By:	Components:		
M. C. Haulait-Pirson	(1) Hexane; C ₆ H ₁₄ ; [110-54-3] (2) Water; H ₂ O; [7732-18-5]		
Variables:	Prepared By:		
One temperature: 25 °C	A. Skrzecz, I. Owczarek, and K. Blazej		
Experimental Data	Experimental Data		
The solubility of water in hexane at 25 °C was reported to be in mole fraction, $x_2 = 5.1 \cdot 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.01066 g(2)/100 g sln.	$t/^\circ\text{C}$	mol(1)/L. sln	x_1 (compiles)
	25.0	$1.43 \cdot 10^{-4}$	$2.58 \cdot 10^{-6}$
	Auxiliary Information		
Method/Apparatus/Procedure:	Source and Purify of Materials:		
The Karl Fischer method was used. The experimental apparatus and procedures are given in Sugi <i>et al.</i> ¹	(1) Merck Uvasol spectrograde chemical; used without further purification. (2) Deionized and fractionated twice in an all-glass distillation flask.		
Estimated Error:	Method/Apparatus/Procedure:		
Not specified.	The generator column method was used as described in DeVoe <i>et al.</i> ² A column was coated with (1) by pulling about 2 ml. of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column. The effluent was then analyzed by gic. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.		
References:	Estimated Error:		
¹ H. Sugi, T. Nitta, and T. Katayama, J. Chem. Eng. Jpn., 9 , 12 (1976).	(1) Source not specified; purity >99 mole % checked by high temperature gic. (2) Source not specified.		
References:	Estimated Error:		
² H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA), 86 , 361 (1981).	Temperature: ± 0.1 °C. Solubility: 1% (estimated by the authors).		
References:	References:		
¹ H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA), 86 , 361 (1981).	H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA), 86 , 361 (1981).		
² W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem., 50 , 175 (1978).	W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem., 50 , 175 (1978).		

Components:	Original Measurements: C. Tsionopoulos and G. M. Wilson, AIChE J. 29 , 990 (1983).	
Variables:	(1) Hexane: C_6H_{14} ; [110-54-3] (2) Water: H_2O ; [7732-18-5]	
Prepared By:	G. T. Hefter	
Experimental Data	The solubility of hexane in water	
T/K	$10^4 \cdot x_1$	P/MPa^a
310.93	0.238	0.114
306.93	0.573	0.274
306.48	0.535	0.256
307.55	0.621	0.297
313.15	2.71	1.30
312.04	3.39	1.62
423.15	18.5	8.85
473.15		3.516
The solubility of water in hexane		
T/K	$10^2 \cdot x_2$	P/MPa^a
313.15	0.117	0.04537
313.15	0.123	— ^a
367.55	0.595	0.124
373.15	0.709	0.148
423.15	3.11	0.667
473.15	11.0	2.52
The solubility of water in hexane		
Components:	Original Measurements: Ya. D. Zelvenskii, A. A. Efremov, and G. M. Larin, Khim. Tekhnol. Topl. Massei 10 , 3 (1965).	
Variables:	One temperature: 20 °C	
Prepared By:	A. Maczynski	
Experimental Data	The solubility of water in hexane at 20 °C was reported to be 0.0166 g(2)/100 g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 7.9·10 ⁻⁴ .	
T/K	$10^2 \cdot g(1)/100 \text{ g sln}$ (compiler)	Auxiliary Information
Method/Apparatus/Procedure:	Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through a vessel with (2) and then through a vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.	
Source and Purity of Materials:	(1) Source not specified; pure grade; shaken with concentration H_2SO_4 ; washed with water, dried over sodium, and distilled; purity not specified. Boiling point 68.81 °C, melting point -95.5 °C. (2) Source not specified; commercial 1 Ci/ml. HTO used as received.	
Estimated Error:	Not specified.	

The three phase critical point was reported to be 496.7 K, 5.295 MPa, and $x_1 = 4.982 \cdot 10^{-4}$ (0.238 g(1)/100 g ln. compiler). Average value.

to their own and literature data over the range 27–
 $x_1 = -367.9847 + 16128.646/T + 52.820813 \ln T$
 $\ln x_2 = -45.1714 - 1635.73/T + 7.53503 \ln T$

Auxiliary Information	Source and Purity of Materials:
Method/Apparatus/Procedure:	All experimental details are given in an Appendix deposited in a Documentation Center rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, while that of (2) in (1) was measured by the Karl Fischer titration.
Source:	(1) No details given. (2) No details given.
Estimated Error:	Temperature: not stated Solubility: $\pm 5\%$ relative; repeatability of replicate analyses Pressure: $\pm 1\%$; type of error not stated

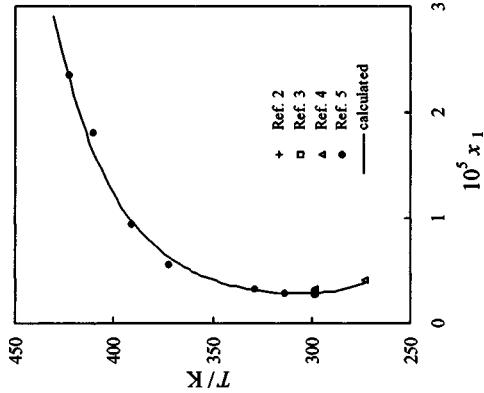


Fig. 7. All the solubility data for 2-methylpentane (1) in water (2).

3.4. 2-Methylpentane*

Components:

(1) 2-Methylpentane: C_5H_{12} ; [107-83-5]
 (2) Water: H_2O ; [7732-18-5]

Critical Evaluation of the Solubility of 2-Methylpentane (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Leinonen and D. Mackay ²	298	Polak and Lu ⁴	273 and 298
McAuliffe ³	298	Price ⁵	298-423

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + \Delta_{\text{sl}} C_p / R [T_{\min} / T - \ln(T_{\min} / T) - 1], \quad (1)$$

where: $\ln x_{1,\min} = -12.87$; $\Delta_{\text{sl}} C_p / R = 44.8$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data.

Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data are listed in Table 9 and shown in Fig. 7. All the data at 298 K are in good agreement with each other and with reference data (within 30% relative standard deviation) and are Recommended. All other data are in good agreement with the reference data and are Tentative.

TABLE 9. Experimental values for solubility of 2-methylpentane (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	4.06·10 ⁻⁶ (T; Ref. 4) 2.72·10 ⁻⁶ (R; Ref. 5), 3.28·10 ⁻⁶ (R; Ref. 3), 3.10·10 ⁻⁶ (R; Ref. 2)	3.8·10 ⁻⁶ 2.9·10 ⁻⁶	273.2 298.2	1.39·10 ⁻⁴ (T; Ref. 4) 4.31·10 ⁻⁴ (D; Ref. 4)
298.2	2.88·10 ⁻⁶ (T; Ref. 5) 3.28·10 ⁻⁶ (T; Ref. 5)	2.9·10 ⁻⁶		1.9·10 ⁻⁴ 2.9·10 ⁻⁴
313.3	5.67·10 ⁻⁶ (T; Ref. 5)	3.2·10 ⁻⁶		
328.9	9.39·10 ⁻⁶ (T; Ref. 5)	6.3·10 ⁻⁶		
372.3	1.81·10 ⁻⁵ (T; Ref. 5)	9.8·10 ⁻⁶		
391.2	2.36·10 ⁻⁵ (T; Ref. 5)	1.6·10 ⁻⁵		
410.5		2.3·10 ⁻⁵		
422.7				

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szlega⁶ are independent data. Therefore these data are Rejected.

References:

- ¹J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).
- ²P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).
- ³C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
- ⁴J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
- ⁵L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
- ⁶T. Krzyzanowska and J. Szlega, Nauk. Katowicei **12**, 413 (1978).

Polak and Lu⁴ investigated the experimental solubility data for (2) in (1) at 273 K and 298 K. Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_1 - 1) + d_3(1 - T_1)^3 + d_4(1 - T_1), \quad (2)$$

where: $d_1 = -1.207$; $d_2 = -6.227$; $d_3 = -0.065$; $d_4 = -5.204$; $T_1 = T/491.7$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 2-methylpentane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 10. The data of Polak and Lu² at 273 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Polak and Lu² at 298 K are in poor agreement with the reference data and are Doubtful.

High Pressure Solubility of 2-Methylpentane (1) in Water (2)

Connolly¹ has investigated the high pressure solubility for (1) in (2) at constant temperatures 573 K–628 K and 14 180 KPa–70 910 kPa. The data measured by one author only have not been critically evaluated.

TABLE 10. Experimental values for solubility of water (2) in 2-methylpentane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	1.39·10 ⁻⁴ (T; Ref. 4) 4.31·10 ⁻⁴ (D; Ref. 4)	1.9·10 ⁻⁴ 2.9·10 ⁻⁴

Auxiliary Information

Components:(1) 2-Methylpentane; C_5H_{12} ; [107-83-5]
(2) Water; H_2O ; [7732-18-5]**Variables:**Temperature: 300 °C–355 °C
Pressure: 140 atm–700 atm**Original Measurements:**

J. F. Connolly, J. Chem. Eng. Data II, 13 (1966).

Prepared By:

M. C. Haulait-Pinson

Method/Apparatus/Procedure:

The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.

Source and Purity of Materials:

(1) Phillips reagent grade; better than 99.8% used as received.
(2) Distilled and deaerated.

Estimated Error:

Temperature: ±0.02 °C.
Pressure: ±2 atm (accuracy).

Auxiliary Information**Experimental Data**

Solubility of 2-methylpentane in water			
t/°C	x_1 (compiler)	g(1)/100 g sln	P/atm
			P/MPa (compiler)
300	0.0023	1.1	14.18
300	0.0027	1.3	27.86
300	0.0027	1.3	48.12
300	0.0027	1.3	70.91
330	0.0038	1.8	16.21
330	0.0058	2.7	18.74
330	0.0084	3.9	21.78
330	0.0086	4.0	24.82
330	0.0091	4.2	30.39
330	0.0089	4.1	41.53
330	0.0080	3.7	50.65
340	0.0097	4.5	21.27
340	0.0118	5.4	23.80
340	0.0138	6.3	26.84
340	0.0152	6.9	30.39
340	0.0140	6.4	37.0
340	0.0116	5.3	48.5
350	0.0157	7.1	23.30
350	0.0183	8.2	24.31
350	0.0237	10.4	26.34
350	0.0267	11.6	27.86
350	0.0290	12.5	29.38
350	0.0297	12.8	31.40
350	0.0290	12.5	33.94
350	0.0267	11.6	36.97
350	0.0239	10.5	41.03
355	0.0303	13.0	24.82
355	0.0353	14.9	24.82
355	0.0421	17.4	25.32
355	0.0526	21.0	25.32
355	0.1109	37.4	385
355	0.1015	35.1	380
355	0.0925	32.8	380
355	0.0829	30.2	380
355	0.0731	27.4	380
355	0.0628	24.3	380
355	0.0526	21.0	385
355	0.0419	17.3	385
			39.00

Comments and additional data:

Upper critical solution temperature: 352 °C at $P=310$ atm.
The uncertainty in the CST is about 2 °C and the corresponding pressure about 10 atm.

Components:	Original Measurements:	Original Measurements:
(1) 2-Methylpentane; C_6H_{14} ; [107-83-5] (2) Water; H_2O ; [7732-18-5]	P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. 51 , 230 (1973).	C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).
Prepared By:	Variables:	Prepared By:
M. C. Haulait-Pirson	One temperature: 25 °C	M. C. Haulait-Pirson
Experimental Data	Auxiliary Information	Experimental Data
The solubility of 2-methylpentane in water at 25 °C was reported to be 14.2 mg(1)/L sln. With the assumption of a solution density of 1.00 g./mL, the corresponding mass percent is 0.00142 g(1)/100 g sln and the corresponding mole fraction, x_1 , is $3.0 \cdot 10^{-6}$ (compiler).		The solubility of 2-methylpentane in water at 25 °C was reported to be 13.8 mg(1)/kg sln (0.00138 g(1)/100 g sln). The corresponding mole fraction, x_1 , calculated by the compiler, is $2.88 \cdot 10^{-6}$. The same value is also reported in McAuliffe, ^{1,2}
Method/Apparatus/Procedure:	Source and Purify of Materials:	Source and Purify of Materials:
Method/Apparatus/Procedure: A mixture of (1) and (2) was equilibrated for at least 12 h in a 200 mL Teflon stopped vessel with gentle shaking. The solution was allowed to settle for 6 h and the aqueous phase was tested (Tyndall effect). Both phases were analyzed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by gic. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.	Source and Purify of Materials: (1) Phillips Petroleum Co.; research grade; purity 99+ % used as received. (2) Doubly distilled.	Source and Purify of Materials: (1) Phillips Petroleum Co.; 99+ % purity; used as received. (2) Distilled.
Estimated Error:	Estimated Error:	Estimated Error:
Estimated Error: Temperature: ± 0.1 °C. Solubility: ± 1 mg(1)/L sln.	Estimated Error: Temperature: ± 1.5 °C. Solubility: 0.9 mg(1)/kg sln (std. dev. of mean).	Temperature: ± 1.5 °C. Solubility: 0.9 mg(1)/kg sln (std. dev. of mean).
References:	References:	References:
		[1] C. McAuliffe, Nature (London) 200 , 1092 (1963). [2] C. McAuliffe, Ann. Chem. Soc. Div. Petrol. Chem. 9 , 275 (1964).

Components:		Original Measurements:		Original Measurements:	
(1) 2-Methylpentane; C ₆ H ₁₄ ; [107-83-5]		J. Polak and B. C.-Y. Lu, Can. J. Chem., 51 , 4018 (1973).		L. C. Price, Am. Assoc. Pet. Geol. Bull., 60 , 213 (1976).	
(2) Water; H ₂ O; [7732-18-5]					
Prepared By:		Prepared By:		Prepared By:	
M. C. Haulait-Pirson		F. Kapuku			
Variables:		Variables:		Variables:	
Temperature: 0 °C–25 °C		Temperature: 25 °C–149.5 °C		Temperature: 25 °C–149.5 °C	
Experimental Data		Experimental Data		Experimental Data	
Solubility of 2-methylpentane in water		Solubility of 2-methylpentane in water at system pressure		Solubility of 2-methylpentane in water at system pressure	
$t/^\circ\text{C}$		$t/^\circ\text{C}$		$t/^\circ\text{C}$	
$10^6 \cdot x_1$ (compiler)		$10^6 \cdot x_1$ (compiler)		$10^6 \cdot x_1$ (compiler)	
0 ^a		19.45 ^c		2.72	
25 ^b		4.06 3.28		2.88 3.28	
		15.7 ^c		0.00130 0.00138	
		55.7		0.00157	
		99.1		0.00271	
		118.0		5.67	
		137.3		9.39	
		149.5		18.15	
		23.62		23.62	
		$10^6 \cdot x_2$ (compiler)		$g(1)/100 \text{ g sln}$ (compiler)	
		mg(1)/kg sln		mg(1)/kg(2)	
		mg(2)/kg sln			
0 ^a		1.39		29 ^d	
25 ^b		2.31		90 ^e	
^{a–e} See Estimated Error.		Auxiliary Information		Auxiliary Information	
Method/Apparatus/Procedure:		Source and Purity of Materials:		Source and Purity of Materials:	
		Room-temperature solubility was determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase.		Source and Purity of Materials:	
		High-temperature solubility work was carried out in the oven of a gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample was then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.		(1) Phillips Petroleum Company; 99+ %. (2) Distilled.	
Method/Apparatus/Procedure:		Source and Purity of Materials:		Estimated Error:	
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.		(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water. (2) Distilled.		(1) Phillips Petroleum Company; 99+ %. (2) Distilled.	
Estimated Error:		Estimated Error:		Estimated Error:	
		Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C. Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).		Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C. Solubility: (c) ± 1.7%; (d) ± 4.7%; (e) ± 3.1% (mean).	

agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Polak and Lu² at 273 K are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeli⁵ are independent data. These data are therefore Rejected.

References:

- ¹C. McAuliffe, J. Phys. Chem., **70**, 1267 (1966).
- ²J. I. Polak and B. C. Y. Lu, Can. J. Chem., **51**, 4018 (1973).
- ³L. C. Price, Am. Assoc. Pet. Geol. Bull., **60**, 213 (1976).
- ⁴E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim., **53**, 1298 (1979).
- ⁵T. Krzyzanowska and J. Szeli⁵, Natta (Katowice) **12**, 413 (1978).

Critical Evaluation of the Solubility of 3-Methylpentane (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
McAuliffe ¹ Polak and Lu ²	298 273 and 298	Price ³ Rudakov and Lutsyk ⁴	298 298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + \Delta_{\text{sln}} C_p / R [T_{\min}/T - \ln(T_{\min}/T) - 1], \quad (1)$$

where: $\ln x_{\min,1} = -12.68$; $\Delta_{\text{sln}} C_p / R = 43.8$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 11. The data of McAuliffe,¹ Price,³ and Rudakov and Lutsyk⁴ are in good agreement with each other and with reference data (within 30% relative standard deviation) and are Recommended. The data of Polak and Lu² are in poor agreement with reference data and are Doubtful.

TABLE 11. Experimental values for solubility of 3-methylpentane (1) in water (2)

T/K	Experimental values x_1 (R=recommended, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$4.49 \cdot 10^{-6}$ (D; Ref. 2)	$4.6 \cdot 10^{-6}$
298.2	$2.68 \cdot 10^{-6}$ (R; Ref. 1), $3.74 \cdot 10^{-6}$ (D; Ref. 2), $2.74 \cdot 10^{-6}$ (R; Ref. 3), $2.70 \cdot 10^{-6}$ (R; Ref. 4)	$3.5 \cdot 10^{-6}$

Critical Evaluation of the Solubility of Water (2) in 3-Methylpentane (1)

Polak and Lu² have investigated the experimental solubility for (2) in (1) at 273 K and 298 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2 / (T/T_c - 1) + d_3 (1 - T_c)^3 + d_4 (1 - T_c), \quad (2)$$

where: $d_1 = -1.169$; $d_2 = -6.213$; $d_3 = -0.158$; $d_4 = -4.918$; $T_c = 497.4$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 3-methylpentane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 12. The data of Polak and Lu² at 298 K are in good

TABLE 12. Experimental values for solubility of water (2) in 3-methylpentane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	$1.1 \cdot 10^{-4}$ (D; Ref. 2)	$1.8 \cdot 10^{-4}$
298.2	$4.5 \cdot 10^{-4}$ (T; Ref. 2)	$6.1 \cdot 10^{-4}$

Components:	Original Measurements: C. McAuliffe, J. Phys. Chem., 70 , 1267 (1966).	
(1) 3-Methylpentane; C_6H_{14} ; [96-14-0]		
(2) Water; H_2O ; [7732-18-5]		
Variables:		
One temperature: 25 °C		
Prepared By:		
M. C. Hadjali-Pirson		
Experimental Data		
The solubility of 3-methylpentane in water at 25 °C was reported to be 12.8 mg(1)/kg sln (0.00128 g(1)/100 g sln). The same value is also reported in McAuliffe. ¹		
The corresponding mole fraction, x_1 , calculated by the compiler, is $2.68 \cdot 10^{-6}$.		
Auxiliary Information		
Source and Purity of Materials:		
(1) Phillips Petroleum Co.; 99+ % purity; used as received.		
(2) Distilled.		
Estimated Error:		
Temperature: ± 1.5 °C.		
Solubility: 0.6 mg(1)/kg sln (std. dev. of mean).		
References:		
[C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem., 9 , 275 (1964).]		
a-e See Estimated Error.		
Original Measurements:		
Components:		
(1) 3-Methylpentane; C_6H_{14} ; [96-14-0]		
(2) Water; H_2O ; [7732-18-5]		
Variables:		
Temperature: 0 °C–25 °C		
Prepared By:		
M. C. Hadjali-Pirson		
Experimental Data		
Solubility of 3-methylpentane in water		
$10^6 \cdot x_1$ (compiler)		
t/°C		
0 ^a		
25 ^b		
4.49		
3.74		
$10^4 \cdot x_2$ (compiler)		
t/°C		
0 ^a		
25 ^b		
1.10		
4.50		
mg(1)/kg sln		
21.5 ^c		
17.9 ^c		
Auxiliary Information		
Method/Apparatus/Procedure:		
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.		
Source and Purity of Materials:		
(1) Phillips Petroleum Co.; pure grade reagent 99+ %; shaken three times with distilled water.		
(2) Distilled.		
Estimated Error:		
Temperature: (a) ± 0.02 °C; (b) ± 0.01 °C.		
Solubility: (c) $\pm 1.7\%$; (d) $\pm 4.7\%$; (e) $\pm 3.1\%$ (mean).		

Components:		Original Measurements:	
(1) 3-Methylpentane; C_6H_{14} : [96-14-0]	L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	(1) 3-Methylpentane; C_6H_{14} : [96-14-0]	E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. 53 , 1298 (1979).
(2) Water; H_2O ; [7732-18-5]		(2) Water; H_2O ; [7732-18-5]	
Prepared By:		Experimental Data	
M. C. Haulait-Pirson		The authors reported the partition coefficient α of 3-methylpentane between the gas and aqueous phase, $\alpha = 68 \pm 4$. $\alpha = C_g/C_s$ with C_g being the concentration of the compound in dilute aqueous solution at 25 °C and C_s the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter). The compiler has assumed that when (1) and (2) are not very soluble in each other, C_g may be taken as the water solubility and C_s as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Ref. 1. $P = 189.8$ mm of Hg and $\log C_g = \log P - 4.265 = 1.99$ expressed in moles per liter. Therefore $C_g = 1.50 \cdot 10^{-4}$ moles/L. With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.0013 g/(1/100 g sin and the corresponding mole fraction, x_1 , is $2.7 \cdot 10^{-6}$.	
Variables:		Auxiliary Information	
One temperature: 25 °C			
Experimental Data		Source and Purity of Materials:	
The solubility of 3-methylpentane in water at 25 °C and at system pressure was reported to be 13.1 mg(1)/kg (2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00131 g(1)/100 g sin and $2.74 \cdot 10^{-6}$.		(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.	
Auxiliary Information		(2) Distilled.	
Method/Apparatus/Procedure:		Estimated Error:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.		Temperature: ± 1 °C. Solubility: ± 0.4 mg(1)/kg(2).	The equilibrium distribution was attained after shaking a mixture for 10 m in a thermostatted reactor containing (2) and (1) vapor. After being allowed to stand for 10 m, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.
Estimated Error:		Estimated Error:	
Temperature: ± 1 °C. Solubility: ± 0.4 mg(1)/kg(2).		Solubility: $\pm 10\%$ (estimated by the compiler).	
References:		I. J. Hine and P. K. Mooker, J. Org. Chem. 4 , 292 (1975).	

4. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

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5. Registry Number Index

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